STRUCTURAL CHEMISTRY

Volume 79 (2023)

Supporting information for article:

Structure determination of a bis[4-(di-*n*-butylamino)phenyl](pyridin-3-yl)borane tetramer highlighting a unique geometric conformation of the core 16-membered ring

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S1. NMR Spectra

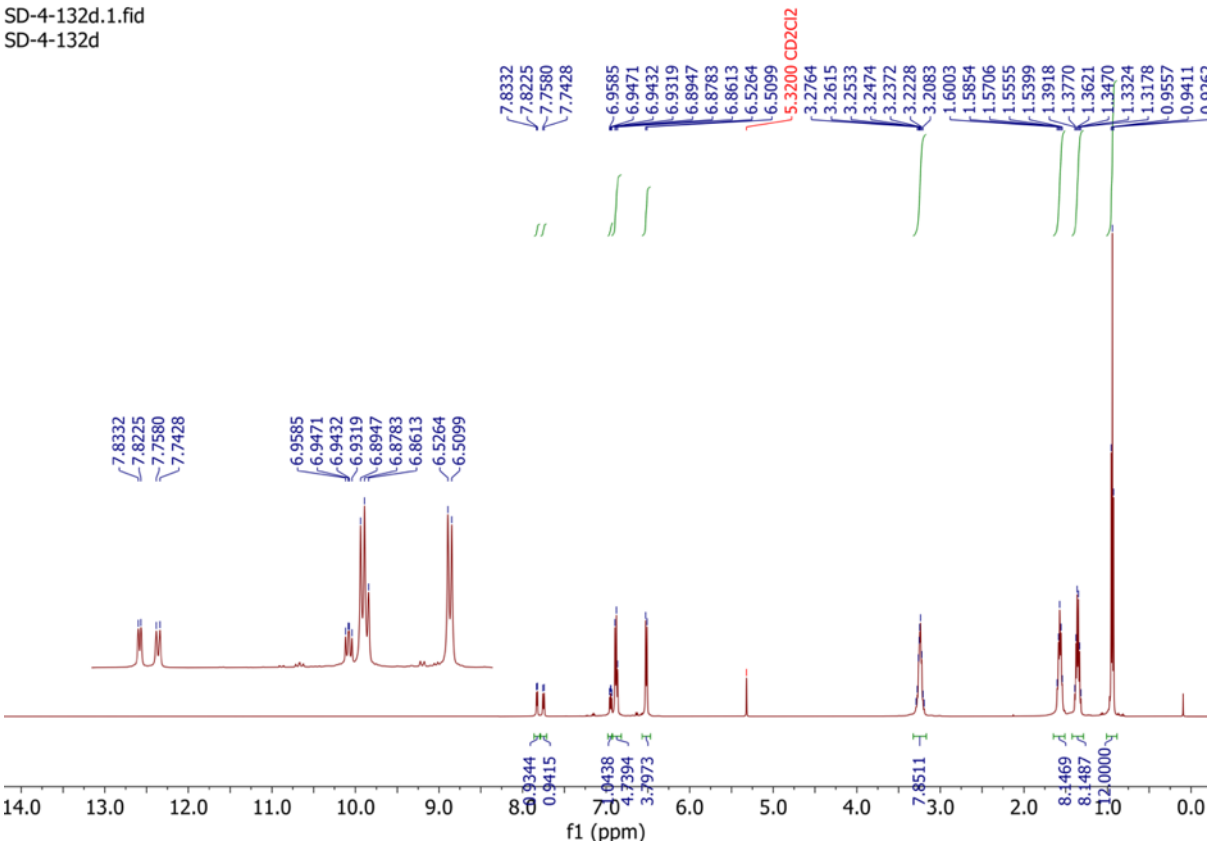

Figure S1 ^{1}H-NMR spectrum of **1** in CD_2Cl_2 collected on a 500 MHz Bruker magnet with an Avance-III console.

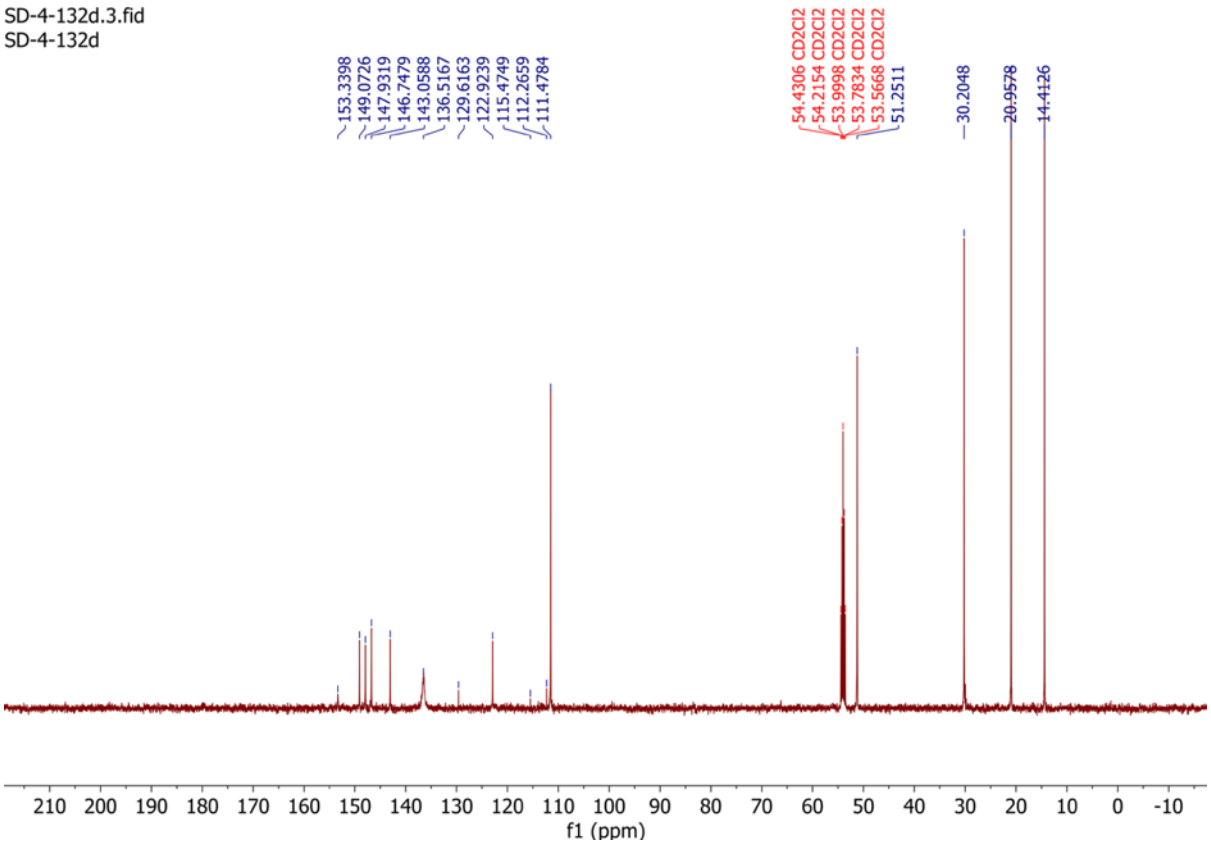

Figure S2 ^{13}C-NMR spectrum of **1** in CD_2Cl_2 collected on a 500 MHz Bruker magnet with an Avance-III console.

S2. Computational details

Twelve compounds were constructed for computations using the methods described in section 2.3. These twelve species are subsequently referred to as **1**-methyl, **1**-phenyl, **1**-2,6-dimethylbenzene, **1**-*tert*-butyl, **2**-methyl, **2**-phenyl, **2**-2,6-dimethylbenzene, **2**-*tert*-butyl, **3**-methyl, **3**-phenyl, **3**-2,6-dimethylbenzene, and **3**-*tert*-butyl. The following tables and figures provide the relevant computational data for each structure. Images were generated using the Mercury software package (Macrae et al., 2020).

Table S1 Atomic coordinates for the optimized structure of **1**-methyl.

Atom Type	X	Y	Z Coordinates
N	-2.813	-1.144	0.001
N	-1.144	2.812	-0.002
N	2.812	1.144	0.001
N	1.144	-2.812	-0.002
C	-2.523	0.947	-1.194
C	-2.372	0.135	-0.071
H	-1.878	0.481	0.836
C	-3.441	-1.692	-1.052
H	-3.764	-2.721	-0.925
C	-3.648	-0.964	-2.218
H	-4.158	-1.429	-3.056
C	-3.185	0.348	-2.283
H	-3.332	0.929	-3.192
C	0.947	2.523	1.194

C	0.135	2.372	0.070
H	0.481	1.879	-0.837
C	-1.693	3.439	1.052
H	-2.721	3.762	0.925
C	-0.965	3.645	2.219
H	-1.430	4.154	3.057
C	0.347	3.183	2.283
H	0.928	3.329	3.193
C	2.523	-0.947	-1.194
C	2.372	-0.135	-0.071
H	1.877	-0.481	0.836
C	3.441	1.692	-1.052
H	3.764	2.721	-0.925
C	3.648	0.964	-2.218
H	4.158	1.429	-3.056
C	3.185	-0.348	-2.283
H	3.333	-0.929	-3.192
C	-0.947	-2.522	1.194
C	-0.347	-3.183	2.283
H	-0.928	-3.329	3.193
C	0.965	-3.645	2.219
H	1.430	-4.154	3.057
C	1.693	-3.439	1.052
H	2.721	-3.762	0.925
C	-0.135	-2.372	0.070
H	-0.482	-1.879	-0.837
B	-2.012	2.475	-1.291
B	2.476	2.012	1.290
B	2.012	-2.475	-1.291
B	-2.476	-2.012	1.290
H	-2.953	3.242	-1.305
H	-1.301	2.622	-2.263
H	2.953	-3.242	-1.305
H	1.301	-2.622	-2.263
H	-3.242	-2.953	1.304
H	-2.623	-1.302	2.262
H	3.242	2.953	1.304
H	2.623	1.302	2.262

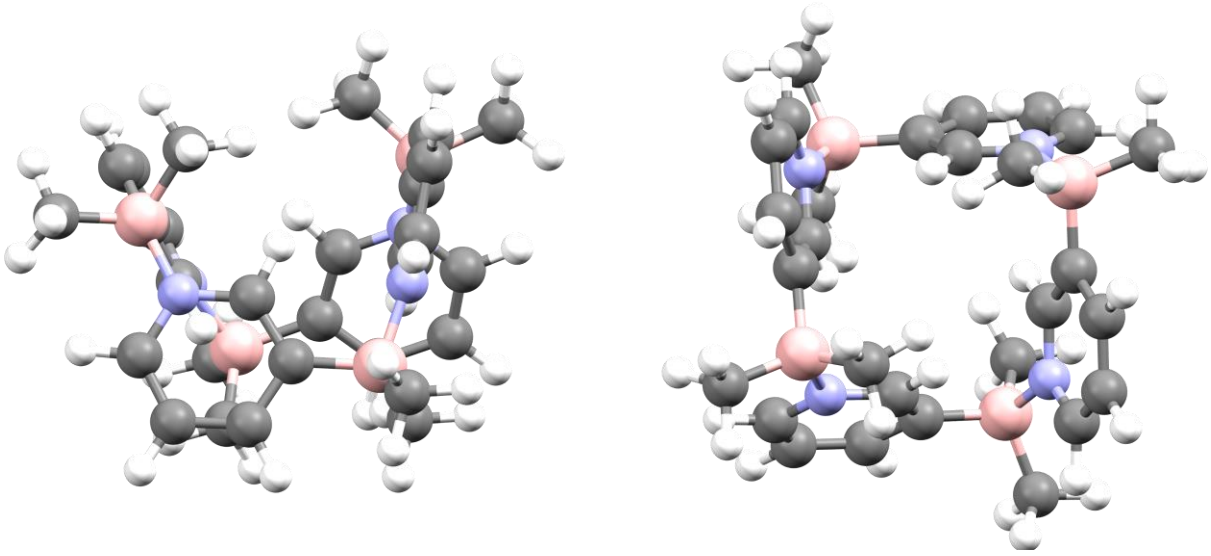

Figure S3 Two views of the optimized structure of **1**-methyl.

Table S2 Atomic coordinates for the optimized structure of **1**-phenyl.

Atom Type	X	Y	Z Coordinates
N	2.850	-0.811	-0.023
N	-0.811	-2.850	0.022
N	-2.850	0.811	-0.022
N	0.811	2.850	0.023
C	1.298	-2.154	-1.325
C	1.671	-1.462	-0.179

H	1.031	-1.420	0.698
C	3.716	-0.774	-1.048
H	4.642	-0.233	-0.882
C	3.432	-1.421	-2.248
H	4.154	-1.376	-3.058
C	2.241	-2.130	-2.372
H	2.037	-2.690	-3.285
C	0.413	-4.623	-1.566
C	1.517	-5.118	-0.839
H	2.058	-4.444	-0.169
C	1.943	-6.442	-0.943
H	2.797	-6.786	-0.361
C	1.279	-7.323	-1.802
C	0.194	-6.859	-2.547
H	-0.324	-7.531	-3.229
C	-0.226	-5.530	-2.428
H	-1.066	-5.190	-3.033
C	-1.117	-2.574	-2.533
C	-2.448	-3.041	-2.482
H	-2.728	-3.754	-1.703
C	-3.423	-2.611	-3.383
H	-4.439	-2.995	-3.308
C	-3.093	-1.688	-4.383
C	-1.787	-1.206	-4.456
H	-1.515	-0.478	-5.221
C	-0.822	-1.643	-3.540
H	0.180	-1.224	-3.610
C	-2.155	-1.299	1.325
C	-1.462	-1.671	0.179
H	-1.419	-1.031	-0.699
C	-0.774	-3.716	1.047
H	-0.234	-4.642	0.881
C	-1.422	-3.433	2.247
H	-1.378	-4.155	3.057
C	-2.131	-2.242	2.371
H	-2.692	-2.038	3.284
C	-4.624	-0.413	1.566
C	-5.118	-1.517	0.838
H	-4.445	-2.058	0.168
C	-6.443	-1.943	0.941
H	-6.787	-2.797	0.359
C	-7.323	-1.279	1.800
C	-6.860	-0.195	2.546
H	-7.531	0.324	3.228
C	-5.530	0.226	2.428
H	-5.191	1.065	3.032
C	-2.574	1.116	2.533
C	-1.644	0.820	3.541
H	-1.225	-0.182	3.610
C	-1.207	1.785	4.458
H	-0.479	1.512	5.222
C	-1.689	3.091	4.384
C	-2.611	3.422	3.384
H	-2.995	4.438	3.309
C	-3.040	2.447	2.483
H	-3.753	2.727	1.703
C	-1.299	2.155	-1.324
C	-1.671	1.462	-0.178
H	-1.031	1.419	0.699
C	-3.716	0.774	-1.047
H	-4.642	0.234	-0.881
C	-3.433	1.423	-2.247
H	-4.155	1.379	-3.056
C	-2.242	2.132	-2.371
H	-2.038	2.693	-3.283
C	1.116	2.574	-2.533
C	0.820	1.645	-3.540
H	-0.182	1.226	-3.610
C	1.785	1.208	-4.458
H	1.512	0.481	-5.222
C	3.091	1.690	-4.384
C	3.422	2.611	-3.383
H	4.438	2.995	-3.308
C	2.447	3.040	-2.482
H	2.728	3.753	-1.702
C	-0.413	4.624	-1.564
C	0.227	5.531	-2.426
H	1.066	5.191	-3.030
C	-0.193	6.861	-2.544
H	0.325	7.532	-3.226

C	-1.277	7.324	-1.798
C	-1.942	6.443	-0.940
H	-2.796	6.787	-0.358
C	-1.516	5.118	-0.837
H	-2.058	4.445	-0.167
C	2.155	1.298	1.325
C	2.131	2.241	2.372
H	2.692	2.037	3.284
C	1.422	3.432	2.248
H	1.378	4.154	3.058
C	0.774	3.716	1.049
H	0.234	4.641	0.883
C	1.462	1.671	0.179
H	1.419	1.031	-0.699
C	4.624	0.412	1.565
C	5.531	-0.227	2.426
H	5.192	-1.067	3.030
C	6.861	0.193	2.545
H	7.532	-0.326	3.226
C	7.323	1.278	1.800
C	6.443	1.943	0.941
H	6.786	2.797	0.360
C	5.118	1.517	0.838

H	4.444	2.058	0.168
C	2.574	-1.117	2.533
C	3.041	-2.448	2.481
H	3.754	-2.728	1.702
C	2.612	-3.423	3.382
H	2.996	-4.439	3.307
C	1.690	-3.093	4.383
C	1.207	-1.787	4.457
H	0.480	-1.515	5.221
C	1.644	-0.822	3.540
H	1.225	0.181	3.610
B	-0.048	-3.070	-1.410
B	-3.070	0.048	1.409
B	0.048	3.071	-1.409
B	3.071	-0.049	1.409
H	8.356	1.608	1.891
H	1.609	-8.355	-1.894
H	1.352	-3.848	5.090
H	-1.607	8.356	-1.890
H	3.845	1.352	-5.092
H	-3.848	-1.350	-5.090
H	-1.351	3.846	5.092
H	-8.356	-1.609	1.892

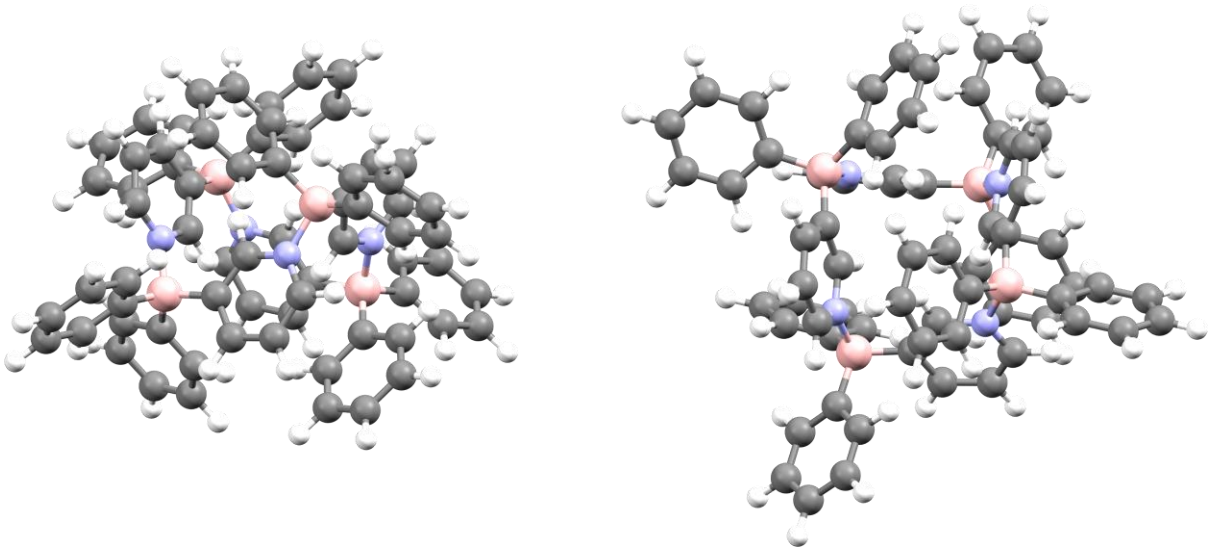

Figure S4 Two views of the optimized structure of **1**-phenyl.

Table S3 Atomic coordinates for the optimized structure of **1**-2,6-dimethylbenzene.

Atom Type	X	Y	Z Coordinates
N	2.843	-1.395	-0.114
N	-1.395	-2.842	0.114
N	-2.843	1.395	-0.114
N	1.395	2.842	0.115
C	1.040	-2.730	-1.066
C	1.536	-1.774	-0.182
H	0.904	-1.311	0.575
C	3.709	-1.932	-0.983
H	4.743	-1.633	-0.883
C	3.326	-2.903	-1.893
H	4.072	-3.345	-2.545
C	2.012	-3.330	-1.892
H	1.718	-4.147	-2.546
C	-0.228	-5.000	-1.126
C	0.329	-5.596	0.039
C	0.528	-6.980	0.132
H	0.934	-7.388	1.056
C	0.242	-7.819	-0.931
C	-0.197	-7.248	-2.118
H	-0.365	-7.882	-2.985
C	-0.416	-5.870	-2.241
C	-1.414	-2.819	-2.465
C	-2.772	-3.242	-2.539
C	-3.612	-2.833	-3.579
H	-4.639	-3.192	-3.597
C	-3.157	-2.003	-4.592
C	-1.832	-1.603	-4.560
H	-1.444	-0.987	-5.368
C	-0.963	-1.991	-3.529
C	-2.730	-1.040	1.067
C	-1.774	-1.536	0.183
H	-1.311	-0.903	-0.575
C	-1.930	-3.708	0.984
H	-1.631	-4.742	0.885
C	-2.902	-3.326	1.894
H	-3.343	-4.072	2.546
C	-3.329	-2.012	1.892
H	-4.147	-1.717	2.546
C	-5.001	0.228	1.126
C	-5.597	-0.329	-0.039
C	-6.980	-0.529	-0.132
H	-7.389	-0.935	-1.056
C	-7.820	-0.243	0.931
C	-7.248	0.195	2.118
H	-7.882	0.363	2.986
C	-5.871	0.415	2.241
C	-2.820	1.415	2.465
C	-1.992	0.964	3.529
C	-1.603	1.833	4.559
H	-0.987	1.447	5.367
C	-2.003	3.159	4.590
C	-2.834	3.613	3.578
H	-3.193	4.640	3.596
C	-3.243	2.772	2.538
C	-1.040	2.730	-1.067
C	-1.536	1.774	-0.182
H	-0.904	1.311	0.575
C	-3.709	1.931	-0.983
H	-4.743	1.632	-0.884
C	-3.326	2.902	-1.894
H	-4.072	3.343	-2.546
C	-2.012	3.329	-1.892
H	-1.717	4.146	-2.547
C	1.414	2.819	-2.465
C	0.964	1.991	-3.529
C	1.832	1.603	-4.559
H	1.446	0.987	-5.367
C	3.158	2.004	-4.591
C	3.612	2.834	-3.579
H	4.639	3.193	-3.597
C	2.772	3.242	-2.539
C	0.228	5.000	-1.126
C	0.416	5.870	-2.241
C	0.197	7.247	-2.118
H	0.365	7.882	-2.985

C	-0.242	7.819	-0.931
C	-0.528	6.979	0.132
H	-0.935	7.388	1.056
C	-0.329	5.596	0.039
C	2.730	1.039	1.067
C	3.328	2.012	1.893
H	4.145	1.717	2.548
C	2.901	3.325	1.894
H	3.342	4.071	2.547
C	1.930	3.708	0.984
H	1.631	4.742	0.885
C	1.774	1.535	0.183
H	1.311	0.903	-0.575
C	5.001	-0.227	1.126
C	5.870	-0.413	2.242
C	7.248	-0.193	2.119
H	7.882	-0.360	2.986
C	7.819	0.245	0.931
C	6.980	0.530	-0.132
H	7.388	0.936	-1.056
C	5.596	0.329	-0.039
C	2.820	-1.415	2.465
C	3.245	-2.772	2.539
C	2.835	-3.613	3.579
H	3.195	-4.640	3.596
C	2.003	-3.160	4.590
C	1.602	-1.835	4.558
H	0.985	-1.449	5.365
C	1.991	-0.965	3.528
B	-0.486	-3.353	-1.188
B	-3.354	0.486	1.188
B	0.486	3.353	-1.188
B	3.354	-0.486	1.188
H	8.892	0.397	0.854
H	0.393	-8.892	-0.853
H	1.694	-3.818	5.397
H	-0.393	8.892	-0.853
H	3.815	1.695	-5.400
H	-3.814	-1.694	-5.400
H	-1.694	3.816	5.398

H	-8.893	-0.395	0.853
C	-5.424	0.790	3.643
H	-4.522	0.257	3.955
H	-5.207	1.857	3.752
H	-6.220	0.540	4.351
C	-4.837	-0.809	-1.265
H	-3.759	-0.671	-1.236
H	-5.015	-1.881	-1.391
H	-5.204	-0.323	-2.178
C	-4.207	3.416	1.562
H	-4.723	4.248	2.050
H	-3.685	3.832	0.692
H	-4.971	2.724	1.201
C	-1.541	-0.468	3.726
H	-0.947	-0.870	2.899
H	-0.930	-0.539	4.627
H	-2.390	-1.140	3.877
C	-3.416	-4.204	-1.562
H	-4.249	-4.720	-2.050
H	-2.725	-4.969	-1.201
H	-3.832	-3.682	-0.692
C	0.470	-1.540	-3.726
H	0.540	-0.929	-4.626
H	0.871	-0.946	-2.898
H	1.141	-2.389	-3.877
C	-0.469	1.540	-3.725
H	-0.539	0.928	-4.626
H	-0.870	0.945	-2.898
H	-1.141	2.388	-3.877
C	3.416	4.205	-1.561
H	3.832	3.682	-0.691
H	4.249	4.720	-2.049
H	2.724	4.969	-1.200
C	4.837	0.808	-1.265
H	3.758	0.671	-1.235
H	5.014	1.881	-1.392
H	5.203	0.321	-2.178
C	5.423	-0.788	3.644
H	4.522	-0.256	3.955
H	5.208	-1.855	3.753

H	6.219	-0.537	4.351
C	4.209	-3.415	1.563
H	4.726	-4.247	2.052
H	3.688	-3.832	0.693
H	4.973	-2.723	1.203
C	1.539	0.467	3.725
H	0.945	0.869	2.898
H	0.927	0.537	4.625
H	2.387	1.139	3.877
C	-0.810	4.836	1.264
H	-1.883	5.012	1.388
H	-0.670	3.758	1.236
H	-0.326	5.205	2.178
C	0.792	5.423	-3.643
H	1.858	5.206	-3.752
H	0.258	4.522	-3.956
H	0.542	6.219	-4.351
C	0.810	-4.836	1.264
H	1.884	-5.010	1.386
H	0.669	-3.758	1.236
H	0.328	-5.206	2.178
C	-0.791	-5.423	-3.643
H	-1.858	-5.207	-3.752
H	-0.258	-4.522	-3.956
H	-0.542	-6.220	-4.351

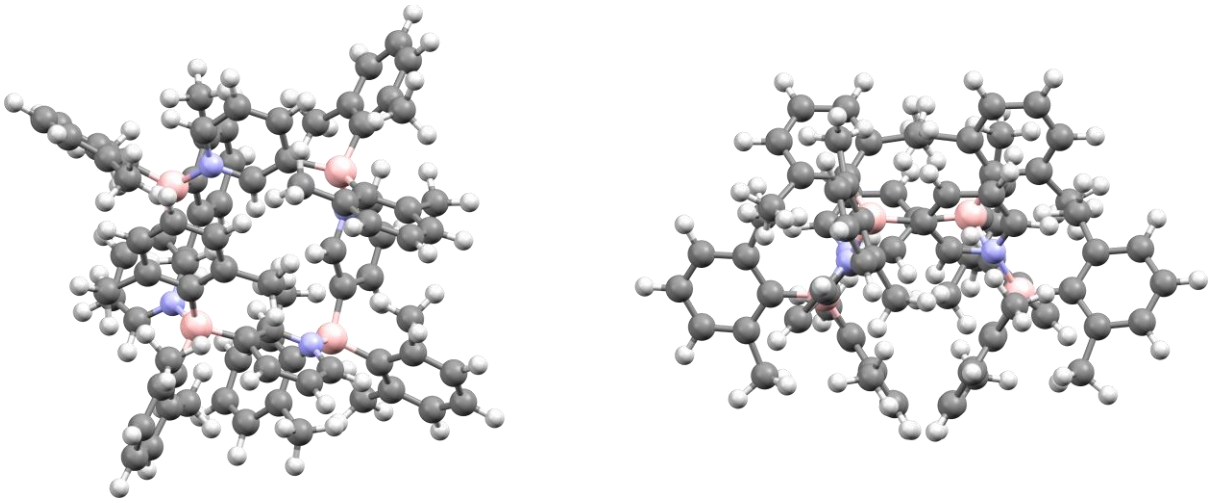

Figure S5 Two views of the optimized structure of **1**-2,6-dimethylbenzene.

Table S4 Atomic Coordinates for the optimized structure of **1**-*tert*-butyl.

Atom Type	X	Y	Z Coordinates
N	-2.711	-1.302	0.094
N	1.301	-2.711	-0.094
N	2.711	1.302	0.094
N	-1.301	2.711	-0.094
C	-0.883	-2.369	1.332
C	-1.435	-1.748	0.209
H	-0.839	-1.601	-0.678
C	-3.508	-1.463	1.163
H	-4.537	-1.170	1.064
C	-3.042	-1.976	2.365
H	-3.720	-2.035	3.209
C	-1.728	-2.408	2.453
H	-1.361	-2.804	3.395
C	2.369	-0.882	-1.332
C	1.748	-1.435	-0.209
H	1.601	-0.838	0.678
C	1.463	-3.508	-1.163

H	1.170	-4.537	-1.064
C	1.976	-3.042	-2.365
H	2.035	-3.720	-3.209
C	2.408	-1.728	-2.453
H	2.804	-1.361	-3.395
C	0.882	2.369	1.332
C	1.435	1.748	0.209
H	0.839	1.601	-0.678
C	3.508	1.463	1.163
H	4.537	1.170	1.064
C	3.042	1.976	2.365
H	3.720	2.035	3.209
C	1.728	2.408	2.453
H	1.361	2.804	3.395
C	-2.369	0.882	-1.332
C	-2.408	1.728	-2.453
H	-2.803	1.361	-3.395
C	-1.975	3.041	-2.365
H	-2.035	3.720	-3.209
C	-1.463	3.508	-1.163
H	-1.169	4.537	-1.064
C	-1.748	1.435	-0.209
H	-1.601	0.838	0.678
B	0.542	-3.186	1.353
B	3.187	0.542	-1.353
B	-0.542	3.186	1.353
B	-3.187	-0.542	-1.353
C	4.831	0.149	-1.246
C	5.738	1.398	-1.117
C	5.115	-0.869	-0.107
C	5.414	-0.611	-2.466
H	5.786	1.935	-2.070
H	5.422	2.135	-0.373
H	6.767	1.100	-0.867
H	4.762	-1.865	-0.402
H	6.198	-0.952	0.063
H	4.652	-0.668	0.859
H	6.441	-0.919	-2.221
H	4.866	-1.533	-2.687
H	5.475	-0.018	-3.376
C	2.713	1.549	-2.630
C	1.271	1.288	-3.130
C	2.835	3.037	-2.247
C	3.560	1.410	-3.914
H	1.209	0.343	-3.683
H	0.500	1.228	-2.355
H	0.964	2.085	-3.822
H	3.830	3.275	-1.854
H	2.667	3.672	-3.130
H	2.107	3.343	-1.495
H	3.112	2.030	-4.703
H	4.586	1.761	-3.780
H	3.598	0.386	-4.300
C	-0.149	4.831	1.246
C	0.611	5.414	2.466
C	0.869	5.115	0.107
C	-1.399	5.738	1.117
H	0.017	5.475	3.376
H	1.533	4.866	2.688
H	0.919	6.440	2.221
H	0.668	4.651	-0.859
H	0.952	6.198	-0.063
H	1.866	4.762	0.403
H	-1.100	6.767	0.867
H	-2.135	5.422	0.373
H	-1.936	5.785	2.069
C	-1.549	2.713	2.630
C	-3.037	2.834	2.247
C	-1.288	1.271	3.130
C	-1.410	3.560	3.914
H	-3.275	3.830	1.854
H	-3.343	2.107	1.495
H	-3.672	2.667	3.130
H	-0.343	1.209	3.683
H	-2.086	0.964	3.822
H	-1.228	0.500	2.355
H	-2.030	3.112	4.703
H	-0.386	3.598	4.300
H	-1.761	4.586	3.780
C	1.549	-2.713	2.630

C	3.037	-2.834	2.247
C	1.288	-1.270	3.129
C	1.410	-3.560	3.914
H	3.275	-3.830	1.854
H	3.343	-2.107	1.494
H	3.672	-2.667	3.129
H	0.343	-1.209	3.683
H	2.086	-0.963	3.822
H	1.228	-0.500	2.355
H	2.030	-3.111	4.703
H	0.386	-3.597	4.300
H	1.761	-4.586	3.780
C	0.149	-4.831	1.246
C	-0.869	-5.115	0.107
C	1.399	-5.738	1.117
C	-0.611	-5.414	2.466
H	-1.865	-4.762	0.403
H	-0.668	-4.652	-0.859
H	-0.952	-6.198	-0.063
H	1.936	-5.785	2.070
H	1.100	-6.767	0.867
H	2.135	-5.421	0.373
H	-0.918	-6.441	2.221
H	-0.017	-5.475	3.376
H	-1.533	-4.866	2.687
C	-2.713	-1.550	-2.630
C	-1.271	-1.288	-3.130
C	-2.835	-3.037	-2.247
C	-3.560	-1.410	-3.914
H	-1.209	-0.343	-3.683
H	-0.500	-1.229	-2.355
H	-0.964	-2.086	-3.822
H	-3.831	-3.275	-1.854
H	-2.667	-3.672	-3.129
H	-2.108	-3.343	-1.494
H	-3.112	-2.031	-4.703
H	-4.586	-1.761	-3.780
H	-3.597	-0.386	-4.300
C	-4.831	-0.149	-1.246
C	-5.739	-1.398	-1.117
C	-5.115	0.870	-0.107
C	-5.413	0.612	-2.466
H	-5.786	-1.935	-2.070
H	-5.422	-2.135	-0.373
H	-6.767	-1.099	-0.867
H	-4.762	1.866	-0.402
H	-6.198	0.953	0.062
H	-4.652	0.668	0.859
H	-6.440	0.919	-2.221
H	-4.866	1.534	-2.687
H	-5.475	0.018	-3.376

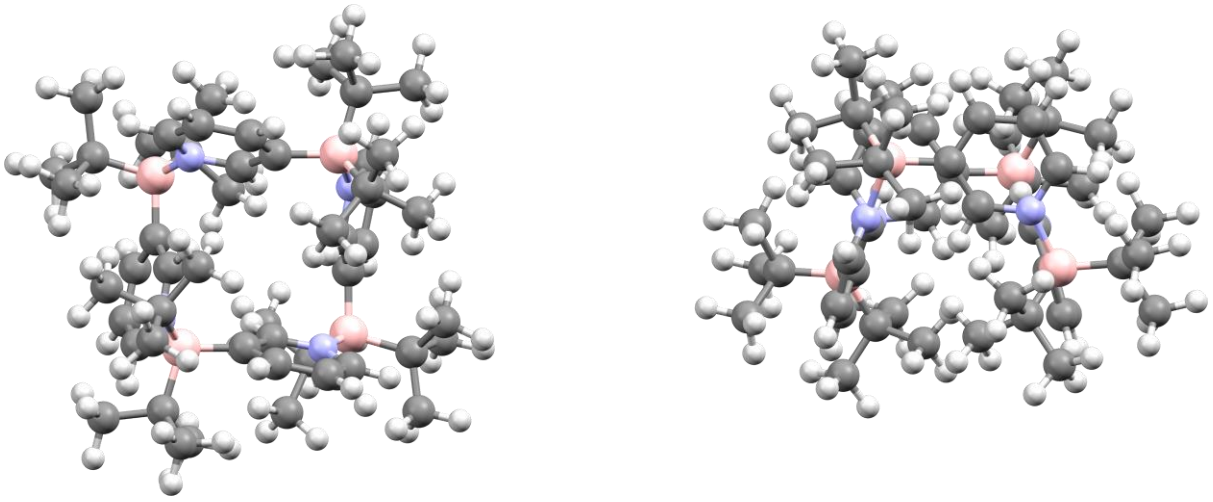

Figure S6 Two views of the optimized structure of **1**-*tert*-butyl.

Table S5 Atomic coordinates for the optimized structure of **2**-methyl.

Atom Type	X Y Z Coordinates		
N	1.450	-2.339	-0.335
N	-3.332	-1.425	0.270
C	0.300	-2.511	0.349
C	-0.975	-2.384	-0.216
C	-1.000	-2.053	-1.579
C	0.181	-1.874	-2.301
C	1.392	-2.023	-1.644
C	-2.870	-0.166	0.420
C	-3.600	0.988	0.132
C	-4.910	0.769	-0.321
C	-5.414	-0.526	-0.461
C	-4.593	-1.606	-0.164
B	-2.333	-2.666	0.648
B	2.932	-2.461	0.361
H	0.420	-2.758	1.399
H	-1.962	-1.931	-2.081
H	0.171	-1.617	-3.357
H	2.348	-1.885	-2.140
H	-1.842	-0.101	0.780
H	-5.540	1.623	-0.570
H	-6.427	-0.706	-0.809
H	-4.924	-2.633	-0.267
B	-2.932	2.461	0.361
C	3.600	-0.988	0.132
N	-1.450	2.339	-0.335
C	2.870	0.166	0.420
C	4.910	-0.769	-0.321
C	-0.300	2.511	0.349
C	-1.392	2.023	-1.644
N	3.332	1.425	0.270
H	1.842	0.101	0.780
C	5.414	0.526	-0.461
H	5.540	-1.622	-0.570
C	0.975	2.384	-0.216
H	-0.420	2.758	1.399
C	-0.181	1.874	-2.301
H	-2.348	1.885	-2.140
C	4.594	1.606	-0.164
B	2.333	2.666	0.648
H	6.427	0.706	-0.809
C	1.000	2.053	-1.579
H	-0.171	1.617	-3.357
H	4.924	2.633	-0.267
H	1.962	1.931	-2.081
C	2.785	-2.746	1.947
H	3.792	-2.779	2.388
H	2.231	-1.969	2.500
H	2.315	-3.717	2.170
C	-2.105	-2.605	2.251
H	-1.609	-1.685	2.601
H	-3.065	-2.676	2.783
H	-1.494	-3.453	2.597
C	-2.984	-4.070	0.164
H	-2.259	-4.875	0.353
H	-3.896	-4.340	0.720
H	-3.219	-4.108	-0.913
C	-2.785	2.746	1.947
H	-2.231	1.969	2.500
H	-2.315	3.717	2.170
H	-3.792	2.779	2.388
C	-3.727	3.647	-0.408
H	-3.916	3.458	-1.478
H	-4.708	3.820	0.062
H	-3.177	4.597	-0.338
C	3.727	-3.647	-0.408
H	4.708	-3.820	0.062
H	3.177	-4.597	-0.338
H	3.916	-3.458	-1.478
C	2.105	2.605	2.251
H	1.609	1.685	2.601
H	3.065	2.676	2.782
H	1.494	3.453	2.597
C	2.984	4.070	0.164
H	2.259	4.875	0.353

H	3.896	4.340	0.720
H	3.218	4.108	-0.914

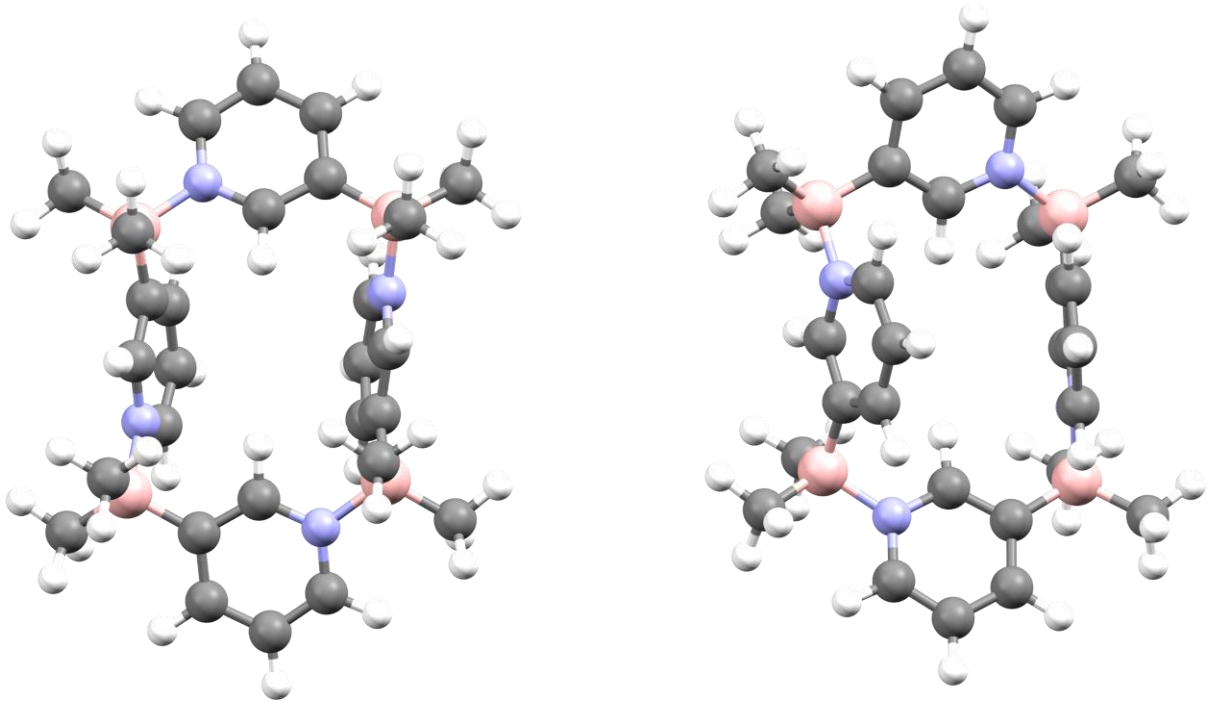

Figure S7 Two views of the optimized structure of **2**-methyl.

Table S6 Atomic coordinates for the optimized structure of **2**-phenyl.

Atom Type	X	Y	Z Coordinates
N	2.089	1.584	-1.064
N	1.842	-3.225	-0.702
C	2.530	0.440	-0.501
C	2.580	-0.791	-1.162
C	2.140	-0.777	-2.495
C	1.726	0.409	-3.107
C	1.706	1.574	-2.359
C	0.572	-2.807	-0.505
C	-0.562	-3.622	-0.565
C	-0.300	-4.960	-0.906
C	1.004	-5.410	-1.120
C	2.062	-4.520	-1.001
B	3.052	-2.163	-0.402
B	2.054	2.996	-0.242
H	2.827	0.527	0.538
H	2.114	-1.710	-3.060
H	1.404	0.433	-4.144
H	1.387	2.529	-2.768
H	0.485	-1.744	-0.289
H	-1.125	-5.659	-1.020
H	1.207	-6.444	-1.384
H	3.096	-4.811	-1.148
B	-2.054	-2.996	-0.242
C	0.562	3.622	-0.565
N	-2.088	-1.583	-1.064
C	-0.572	2.807	-0.505
C	0.300	4.960	-0.904
C	-2.530	-0.440	-0.501
C	-1.707	-1.574	-2.359
N	-1.842	3.225	-0.702
H	-0.485	1.744	-0.289
C	-1.004	5.410	-1.118
H	1.125	5.659	-1.018
C	-2.580	0.791	-1.162
H	-2.827	-0.527	0.538

C	-1.726	-0.409	-3.107
H	-1.388	-2.529	-2.768
C	-2.062	4.520	-0.999
B	-3.052	2.163	-0.402
H	-1.207	6.444	-1.381
C	-2.141	0.777	-2.495
H	-1.406	-0.433	-4.145
H	-3.096	4.811	-1.146
H	-2.115	1.710	-3.060
C	3.134	-1.979	1.211
C	2.271	-2.574	2.143
C	4.165	-1.170	1.737
C	2.401	-2.356	3.522
H	1.471	-3.238	1.812
C	4.302	-0.938	3.103
H	4.881	-0.715	1.049
C	3.413	-1.531	4.007
H	1.705	-2.835	4.208
H	5.098	-0.290	3.465
H	3.513	-1.349	5.075
C	4.454	-2.747	-0.991
C	5.185	-3.684	-0.231
C	5.004	-2.386	-2.232
C	6.375	-4.249	-0.692
H	4.810	-3.969	0.753
C	6.201	-2.938	-2.705
H	4.507	-1.640	-2.851
C	6.889	-3.877	-1.938
H	6.908	-4.970	-0.074
H	6.597	-2.625	-3.669
H	7.821	-4.307	-2.299
C	-2.223	-2.670	1.353
C	-1.255	-1.937	2.073
C	-3.369	-3.048	2.075
C	-1.403	-1.625	3.425
H	-0.355	-1.571	1.580
C	-3.527	-2.753	3.434
H	-4.167	-3.586	1.567
C	-2.541	-2.045	4.119
H	-0.627	-1.053	3.931

H	-4.429	-3.072	3.952
H	-2.662	-1.805	5.173
C	-3.246	-3.932	-0.823
C	-3.439	-5.216	-0.269
C	-4.147	-3.553	-1.831
C	-4.444	-6.078	-0.710
H	-2.797	-5.536	0.554
C	-5.163	-4.404	-2.282
H	-4.081	-2.560	-2.277
C	-5.312	-5.674	-1.730
H	-4.557	-7.058	-0.252
H	-5.843	-4.065	-3.062
H	-6.100	-6.338	-2.077
C	-3.134	1.978	1.211
C	-2.271	2.574	2.143
C	-4.164	1.170	1.737
C	-2.401	2.355	3.522
H	-1.472	3.239	1.812
C	-4.302	0.937	3.103
H	-4.880	0.714	1.049
C	-3.412	1.530	4.007
H	-1.705	2.836	4.208
H	-5.097	0.289	3.465
H	-3.512	1.348	5.075
C	-4.454	2.747	-0.991
C	-5.185	3.684	-0.231
C	-5.004	2.387	-2.232
C	-6.376	4.249	-0.691
H	-4.810	3.969	0.753
C	-6.201	2.938	-2.704
H	-4.507	1.641	-2.851
C	-6.890	3.877	-1.937
H	-6.908	4.969	-0.073
H	-6.598	2.625	-3.668
H	-7.822	4.307	-2.298
C	2.224	2.669	1.353
C	1.256	1.938	2.074
C	3.370	3.047	2.074
C	1.404	1.624	3.425
H	0.355	1.573	1.581

C	3.528	2.751	3.434
H	4.168	3.585	1.566
C	2.542	2.044	4.118
H	0.627	1.053	3.931
H	4.432	3.070	3.951
H	2.664	1.803	5.173
C	3.245	3.933	-0.823
C	3.439	5.216	-0.269
C	4.146	3.554	-1.832
C	4.443	6.078	-0.710
H	2.798	5.536	0.555
C	5.162	4.405	-2.284
H	4.080	2.561	-2.279
C	5.311	5.676	-1.730
H	4.556	7.059	-0.251
H	5.841	4.068	-3.064
H	6.099	6.340	-2.078

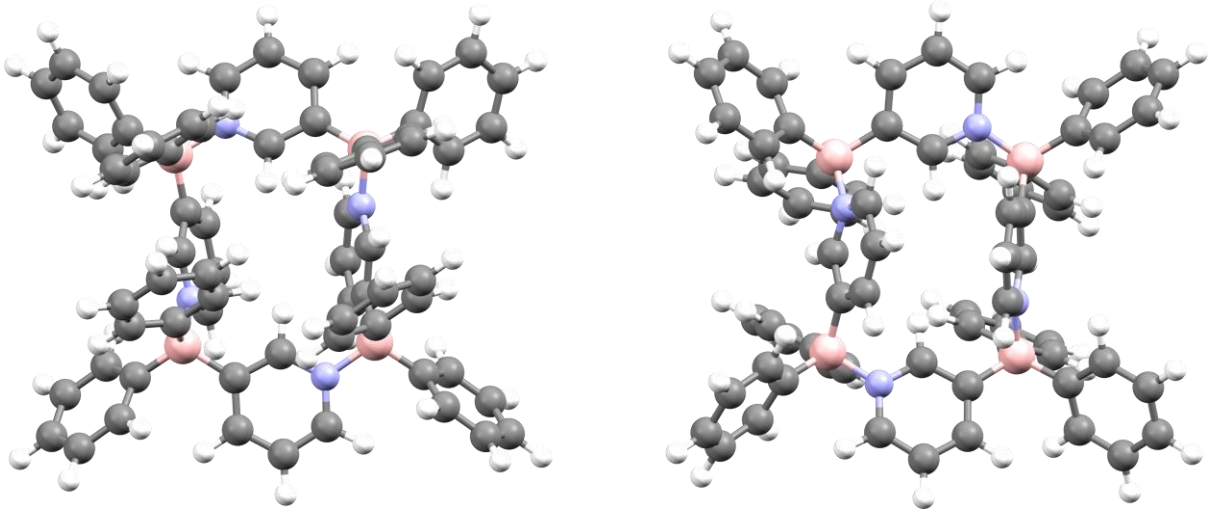

Figure S8 Two views of the optimized structure of **2**-phenyl.

Table S7 Atomic coordinates for the optimized structure of **2**-2,6-dimethylbenzene.

Atom Type	X	Y	Z Coordinates
N	2.229	1.635	-1.107
N	2.231	-3.078	-0.567
C	2.742	0.569	-0.460
C	2.908	-0.698	-1.020
C	2.492	-0.810	-2.352
C	2.057	0.302	-3.067
C	1.927	1.512	-2.409
C	0.951	-2.728	-0.264
C	-0.180	-3.542	-0.426
C	0.135	-4.807	-0.967
C	1.428	-5.167	-1.327
C	2.463	-4.272	-1.128
B	3.481	-2.032	-0.203
B	1.907	3.045	-0.298
H	2.994	0.759	0.575
H	2.553	-1.776	-2.854
H	1.805	0.238	-4.121
H	1.571	2.405	-2.911
H	0.860	-1.718	0.122
H	-0.649	-5.527	-1.160
H	1.635	-6.134	-1.774
H	3.489	-4.489	-1.400
B	-1.821	-3.022	-0.290
C	0.370	3.452	-0.858
N	-1.752	-1.510	-0.946
C	-0.808	2.995	-0.284
C	0.165	4.281	-1.981
C	-2.407	-0.456	-0.395
C	-1.079	-1.328	-2.093
N	-2.056	3.254	-0.733
H	-0.802	2.354	0.580
C	-1.111	4.637	-2.405
H	1.022	4.688	-2.513
C	-2.503	0.812	-0.978
H	-2.862	-0.672	0.563
C	-1.118	-0.122	-2.761
H	-0.554	-2.191	-2.487
C	-2.216	4.096	-1.762
B	-3.230	2.173	-0.274
H	-1.259	5.308	-3.245
C	-1.837	0.929	-2.209

H	-0.606	-0.019	-3.711
H	-3.236	4.281	-2.082
H	-1.867	1.867	-2.759
C	3.480	-1.761	1.432
C	2.715	-2.424	2.436
C	4.273	-0.665	1.881
C	2.578	-1.848	3.711
C	4.119	-0.120	3.158
C	3.230	-0.679	4.066
H	1.957	-2.357	4.445
H	4.700	0.758	3.434
H	3.080	-0.231	5.044
C	4.930	-2.619	-0.808
C	5.507	-3.779	-0.203
C	5.691	-2.055	-1.875
C	6.667	-4.380	-0.700
C	6.855	-2.684	-2.346
C	7.341	-3.854	-1.791
H	7.049	-5.271	-0.207
H	7.396	-2.223	-3.169
H	8.240	-4.325	-2.177
C	-2.682	-2.885	1.144
C	-2.133	-2.775	2.443
C	-4.107	-2.992	1.095
C	-2.901	-3.007	3.592
C	-4.857	-3.197	2.258
C	-4.258	-3.268	3.509
H	-2.413	-2.960	4.564
H	-5.937	-3.305	2.169
H	-4.847	-3.467	4.400
C	-2.649	-4.144	-1.206
C	-2.813	-5.413	-0.571
C	-3.212	-4.017	-2.503
C	-3.462	-6.471	-1.214
C	-3.849	-5.104	-3.121
C	-3.978	-6.332	-2.495
H	-3.563	-7.419	-0.691
H	-4.274	-4.963	-4.113
H	-4.482	-7.159	-2.988
C	-3.276	1.952	1.365
C	-2.501	2.591	2.372
C	-4.129	0.901	1.816
C	-2.425	2.045	3.665
C	-4.020	0.370	3.101
C	-3.126	0.907	4.023
H	-1.793	2.547	4.396
H	-4.647	-0.473	3.379
H	-3.027	0.476	5.016
C	-4.655	2.674	-0.949
C	-5.244	3.868	-0.441
C	-5.371	2.014	-1.986
C	-6.461	4.351	-0.934
C	-6.591	2.523	-2.453
C	-7.146	3.684	-1.938
H	-6.875	5.263	-0.512
H	-7.116	1.984	-3.238
H	-8.095	4.059	-2.311
C	1.951	2.725	1.334
C	1.094	1.760	1.939
C	2.787	3.448	2.236
C	0.934	1.686	3.328
C	2.592	3.362	3.621
C	1.638	2.522	4.177
H	0.254	0.940	3.735
H	3.227	3.957	4.274
H	1.494	2.475	5.253
C	2.874	4.262	-0.850
C	2.458	5.597	-0.598
C	4.061	4.101	-1.605
C	3.118	6.683	-1.178
C	4.700	5.206	-2.184
C	4.221	6.496	-2.003
H	2.768	7.690	-0.961
H	5.606	5.045	-2.764
H	4.726	7.344	-2.458
C	1.330	5.956	0.357
H	1.639	6.805	0.976
H	0.421	6.260	-0.176
H	1.062	5.140	1.030
C	4.790	2.778	-1.751
H	4.766	2.200	-0.822
H	4.387	2.146	-2.549
H	5.842	2.962	-1.990
C	5.426	-0.743	-2.599
H	4.740	-0.861	-3.444
H	5.022	0.041	-1.963
H	6.370	-0.368	-3.007
C	4.929	-4.445	1.022
H	4.941	-3.772	1.883
H	3.897	-4.766	0.877
H	5.511	-5.335	1.277
C	5.390	-0.075	1.043
H	5.652	0.925	1.403
H	6.283	-0.708	1.117
H	5.160	-0.002	-0.018
C	2.163	-3.845	2.383
H	1.915	-4.246	1.404
H	2.915	-4.514	2.818
H	1.274	-3.937	3.007
C	3.982	4.294	1.832
H	4.541	3.853	1.005
H	3.714	5.311	1.532
H	4.661	4.371	2.687
C	0.378	0.627	1.221
H	-0.647	0.521	1.597
H	0.328	0.703	0.133
H	0.912	-0.297	1.476
C	-1.773	3.925	2.257
H	-0.688	3.804	2.366
H	-1.966	4.470	1.338
H	-2.105	4.566	3.082
C	-5.251	0.349	0.963
H	-5.722	-0.497	1.472
H	-6.013	1.116	0.788
H	-4.928	0.002	-0.021
C	-4.601	4.709	0.639
H	-4.432	4.141	1.556
H	-3.635	5.112	0.321
H	-5.240	5.563	0.881
C	-4.937	0.733	-2.675

H	-4.076	0.882	-3.334
H	-4.668	-0.060	-1.975
H	-5.755	0.354	-3.294
C	-2.316	-5.744	0.829
H	-3.076	-5.501	1.581
H	-2.107	-6.817	0.898
H	-1.410	-5.209	1.119
C	-3.287	-2.736	-3.319
H	-3.463	-1.844	-2.717
H	-2.384	-2.563	-3.914
H	-4.119	-2.808	-4.025
C	-0.731	-2.304	2.713
H	-0.752	-1.228	2.926
H	-0.318	-2.788	3.602
H	-0.046	-2.465	1.886
C	-4.947	-2.866	-0.163
H	-4.477	-2.234	-0.921
H	-5.154	-3.836	-0.626
H	-5.907	-2.406	0.092

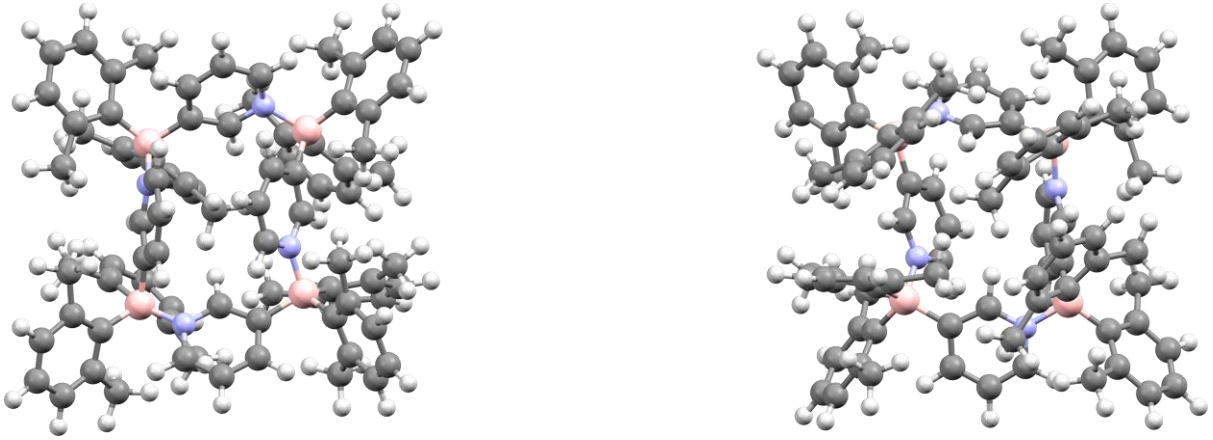

Figure S9 Two views of the optimized structure of **2**-2,6-dimethylbenzene.

Table S8 Atomic coordinates for the optimized structure of **2**-*tert*-butyl.

Atom Type	X	Y	Z Coordinates
N	2.507	1.039	0.796
N	-1.957	3.049	0.010
C	1.750	1.915	0.108
C	0.522	2.438	0.542
C	0.159	2.070	1.841
C	0.953	1.212	2.595
C	2.080	0.669	2.019
C	-2.304	1.743	0.100
C	-3.603	1.256	0.304
C	-4.586	2.252	0.400
C	-4.261	3.600	0.281
C	-2.939	3.962	0.084
B	-0.380	3.508	-0.336
B	3.968	0.358	0.313
H	2.142	2.196	-0.854
H	-0.771	2.438	2.270
H	0.683	0.928	3.606
H	2.665	-0.090	2.517
H	-1.470	1.057	0.002
H	-5.624	1.972	0.563
H	-5.019	4.374	0.339
H	-2.644	4.994	-0.028
B	-3.968	-0.358	0.313
C	3.603	-1.256	0.304
N	-2.507	-1.039	0.796
C	2.304	-1.743	0.100
C	4.586	-2.252	0.400
C	-1.750	-1.915	0.108
C	-2.080	-0.669	2.019
N	1.957	-3.049	0.010
H	1.469	-1.057	0.002
C	4.261	-3.600	0.280
H	5.624	-1.972	0.563
C	-0.522	-2.438	0.542
H	-2.143	-2.196	-0.854

C	-0.953	-1.212	2.595
H	-2.666	0.090	2.517
C	2.939	-3.962	0.083
B	0.380	-3.508	-0.336
H	5.019	-4.373	0.339
C	-0.159	-2.070	1.841
H	-0.683	-0.928	3.606
H	2.644	-4.994	-0.028
H	0.771	-2.438	2.270
C	-0.013	5.033	0.302
C	-0.467	6.268	-0.510
C	-0.515	5.239	1.748
C	1.528	5.164	0.405
H	-0.034	6.289	-1.513
H	-1.552	6.363	-0.631
H	-0.133	7.181	0.002
H	-0.065	4.521	2.440
H	-0.221	6.237	2.102
H	-1.603	5.170	1.860
H	1.795	6.185	0.710
H	1.947	4.487	1.157
H	2.039	4.963	-0.541
C	-0.278	3.326	-2.004
C	1.005	3.904	-2.643
C	-0.350	1.845	-2.422
C	-1.460	4.002	-2.734
H	1.107	4.981	-2.494
H	1.927	3.436	-2.281
H	0.977	3.730	-3.728
H	-1.350	1.438	-2.267
H	-0.128	1.731	-3.493
H	0.348	1.200	-1.880
H	-1.342	3.886	-3.820
H	-2.420	3.539	-2.473
H	-1.537	5.073	-2.529
C	4.339	0.788	-1.270
C	3.217	0.345	-2.240
C	4.646	2.290	-1.479
C	5.570	0.038	-1.841
H	3.301	-0.729	-2.439
H	2.198	0.512	-1.889
H	3.314	0.857	-3.207
H	5.600	2.569	-1.023
H	4.728	2.510	-2.553
H	3.898	2.975	-1.065
H	5.611	0.206	-2.927
H	6.524	0.370	-1.435
H	5.494	-1.046	-1.697
C	5.079	0.835	1.510
C	4.863	2.310	1.914
C	5.048	0.020	2.832
C	6.545	0.749	1.033
H	4.901	2.987	1.054
H	3.901	2.472	2.416
H	5.646	2.626	2.617
H	4.969	-1.062	2.676
H	5.974	0.195	3.396
H	4.240	0.324	3.505
H	7.214	1.020	1.862
H	6.835	-0.254	0.701
H	6.758	1.444	0.219
C	0.278	-3.326	-2.004
C	-1.005	-3.903	-2.643
C	0.350	-1.845	-2.422
C	1.460	-4.001	-2.734
H	-1.107	-4.981	-2.494
H	-1.927	-3.436	-2.281
H	-0.977	-3.729	-3.728
H	1.350	-1.438	-2.268
H	0.127	-1.731	-3.493
H	-0.347	-1.200	-1.880
H	1.342	-3.885	-3.820
H	2.420	-3.539	-2.473
H	1.537	-5.073	-2.529
C	0.013	-5.033	0.301
C	0.467	-6.268	-0.511
C	0.515	-5.239	1.748
C	-1.528	-5.164	0.405
H	0.034	-6.289	-1.513
H	1.552	-6.363	-0.631

H	0.133	-7.181	0.002
H	0.065	-4.521	2.440
H	0.221	-6.237	2.102
H	1.603	-5.169	1.860
H	-1.795	-6.186	0.710
H	-1.947	-4.487	1.157
H	-2.039	-4.963	-0.541
C	-5.078	-0.835	1.510
C	-4.863	-2.311	1.913
C	-5.048	-0.021	2.832
C	-6.545	-0.749	1.034
H	-4.903	-2.987	1.053
H	-3.901	-2.473	2.414
H	-5.646	-2.626	2.617
H	-4.965	1.061	2.676
H	-5.974	-0.194	3.395
H	-4.240	-0.327	3.505
H	-7.214	-1.020	1.862
H	-6.835	0.254	0.702
H	-6.758	-1.444	0.219
C	-4.339	-0.788	-1.270
C	-3.217	-0.345	-2.240
C	-4.646	-2.290	-1.480
C	-5.570	-0.037	-1.841
H	-3.300	0.729	-2.439
H	-2.198	-0.512	-1.889
H	-3.314	-0.857	-3.208
H	-5.601	-2.568	-1.024
H	-4.728	-2.510	-2.553
H	-3.899	-2.975	-1.065
H	-5.611	-0.206	-2.927
H	-6.524	-0.369	-1.435
H	-5.493	1.047	-1.697

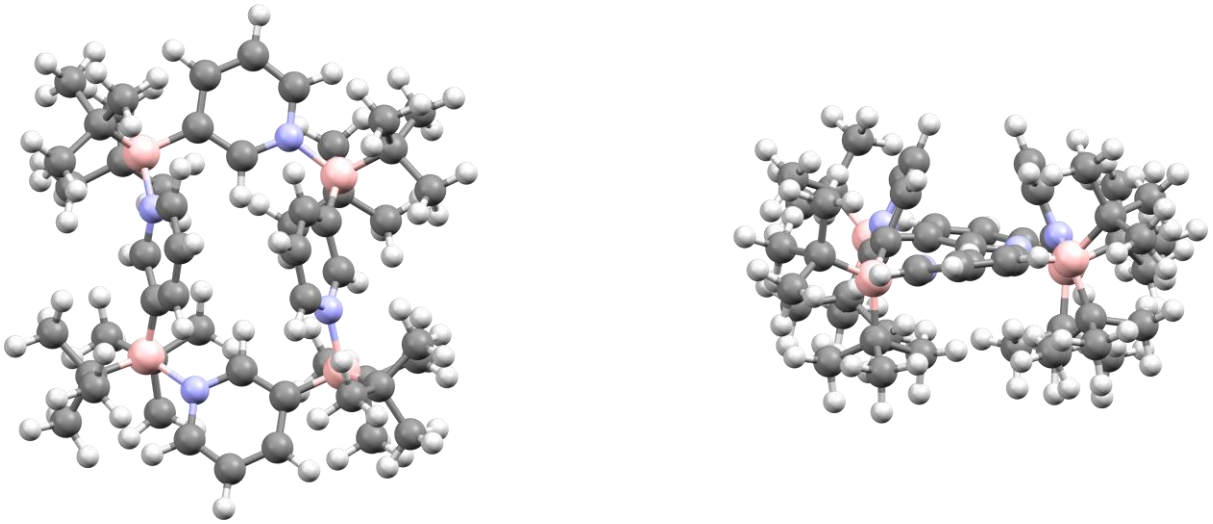

Figure S10 Two views of the optimized structure of **2**-*tert*-butyl.

Table S9 Atomic coordinates for the optimized structure of **3**-methyl.

Atom Type	X Y Z Coordinates		
N	-1.782	-2.320	0.490
N	3.081	-1.707	-0.136
C	-0.656	-2.486	-0.235
C	0.635	-2.476	0.304
C	0.708	-2.264	1.689
C	-0.447	-2.086	2.454
C	-1.680	-2.123	1.820
C	2.763	-0.391	-0.138
C	3.651	0.639	0.167
C	4.953	0.219	0.506
C	5.295	-1.130	0.523
C	4.330	-2.076	0.192
B	1.942	-2.771	-0.626
B	3.254	2.220	0.205
H	-0.811	-2.631	-1.299
H	1.684	-2.235	2.176
H	-0.401	-1.915	3.526
H	-2.613	-1.974	2.352
H	1.726	-0.191	-0.403
H	5.703	0.968	0.760
H	6.297	-1.459	0.784
H	4.538	-3.140	0.178
N	1.782	2.320	-0.489
N	-3.081	1.706	0.135
C	0.656	2.486	0.236
C	-0.635	2.476	-0.304
C	-0.707	2.265	-1.689
C	0.447	2.087	-2.454
C	1.680	2.123	-1.819
C	-2.763	0.391	0.138
C	-3.651	-0.639	-0.167
C	-4.953	-0.219	-0.506
C	-5.295	1.130	-0.524
C	-4.330	2.076	-0.193
B	-1.942	2.771	0.626
B	-3.254	-2.220	-0.205
H	0.811	2.630	1.299
H	-1.683	2.236	-2.176
H	0.402	1.916	-3.525
H	2.614	1.974	-2.352
H	-1.726	0.191	0.404
H	-5.703	-0.968	-0.761
H	-6.296	1.459	-0.785
H	-4.538	3.140	-0.178
C	-2.444	4.290	0.362
H	-2.702	4.499	-0.690
H	-3.305	4.577	0.987
H	-1.629	4.979	0.625

C	-1.691	2.466	2.201
H	-1.267	1.466	2.400
H	-1.005	3.202	2.648
H	-2.633	2.538	2.765
C	3.193	2.720	1.748
H	2.857	3.765	1.841
H	2.569	2.103	2.414
H	4.212	2.682	2.162
C	4.294	3.127	-0.657
H	3.939	4.165	-0.740
H	5.264	3.172	-0.140
H	4.505	2.766	-1.676
C	2.444	-4.290	-0.362
H	3.304	-4.578	-0.987
H	2.702	-4.499	0.690
H	1.628	-4.979	-0.625
C	1.690	-2.466	-2.201
H	1.004	-3.202	-2.648
H	1.267	-1.466	-2.400
H	2.633	-2.538	-2.765
C	-4.294	-3.126	0.658
H	-3.939	-4.165	0.741
H	-4.505	-2.766	1.676
H	-5.264	-3.171	0.141
C	-3.193	-2.721	-1.748
H	-2.857	-3.766	-1.840
H	-4.213	-2.684	-2.161
H	-2.570	-2.104	-2.414

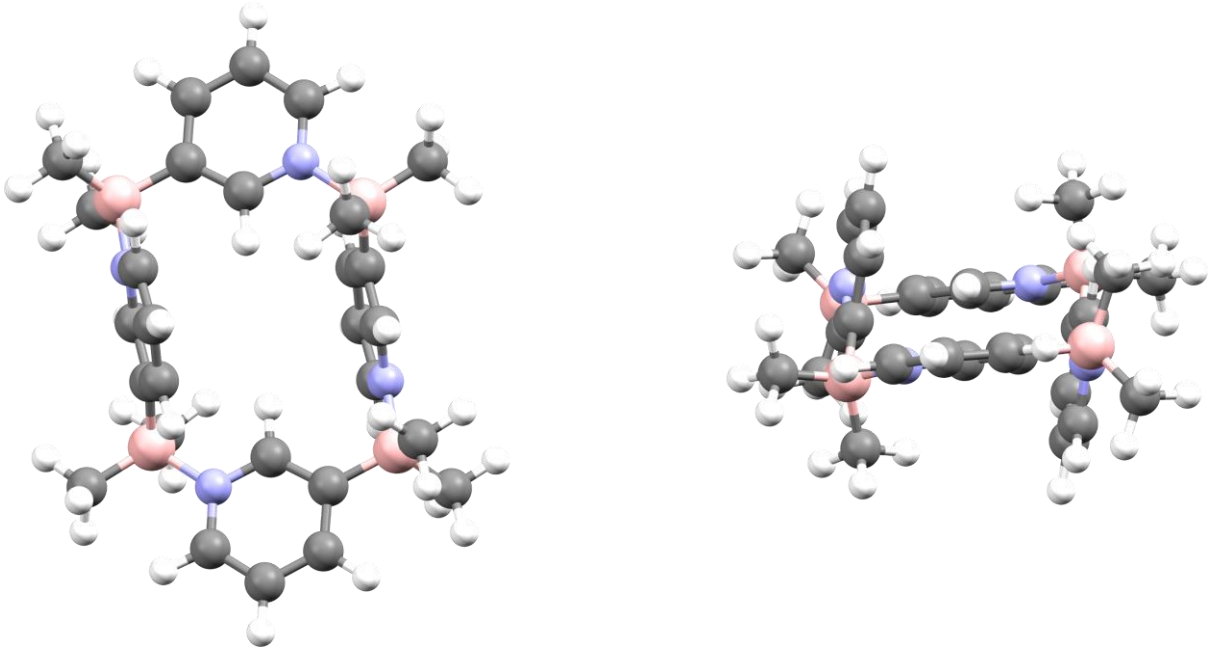

Figure S11 Two views of the optimized structure of **3**-methyl.

Table S10 Atomic coordinates for the optimized structure of **3**-phenyl.

Atom Type	X	Y	Z Coordinates
N	-2.522	0.868	0.824
N	-0.453	-3.587	0.408
C	-2.525	-0.383	0.315
C	-1.920	-1.482	0.932
C	-1.273	-1.207	2.149
C	-1.252	0.083	2.686
C	-1.896	1.098	1.999
C	0.615	-2.783	0.206
C	1.939	-3.217	0.105
C	2.112	-4.607	0.205
C	1.023	-5.453	0.421
C	-0.251	-4.914	0.523

B	-1.960	-2.971	0.250
B	3.171	-2.135	-0.026
H	-3.021	-0.484	-0.643
H	-0.757	-2.011	2.675
H	-0.729	0.309	3.611
H	-1.914	2.126	2.353
H	0.364	-1.730	0.097
H	3.105	-5.037	0.104
H	1.153	-6.528	0.503
H	-1.135	-5.522	0.684
N	2.522	-0.868	-0.824
N	0.453	3.587	-0.408
C	2.525	0.383	-0.315
C	1.920	1.482	-0.932
C	1.274	1.207	-2.149
C	1.253	-0.083	-2.686
C	1.897	-1.098	-1.999
C	-0.615	2.783	-0.206
C	-1.939	3.217	-0.106
C	-2.112	4.607	-0.207
C	-1.024	5.453	-0.423
C	0.250	4.914	-0.525
B	1.960	2.971	-0.250
B	-3.172	2.135	0.025
H	3.021	0.484	0.644
H	0.757	2.011	-2.675
H	0.730	-0.308	-3.612
H	1.914	-2.126	-2.353
H	-0.364	1.730	-0.096
H	-3.106	5.037	-0.106
H	-1.153	6.528	-0.505
H	1.134	5.522	-0.686
C	2.249	2.900	1.351
C	3.559	2.621	1.798
C	1.283	3.104	2.351
C	3.880	2.531	3.151
H	4.351	2.484	1.059
C	1.591	3.014	3.715
H	0.260	3.366	2.078
C	2.892	2.722	4.121
H	4.902	2.306	3.449
H	0.813	3.189	4.457
H	3.138	2.651	5.179
C	3.017	3.947	-1.017
C	3.598	5.043	-0.347
C	3.370	3.786	-2.368
C	4.464	5.933	-0.987
H	3.367	5.199	0.707
C	4.238	4.667	-3.022
H	2.974	2.944	-2.935
C	4.787	5.748	-2.333
H	4.891	6.766	-0.432
H	4.489	4.502	-4.069
H	5.466	6.434	-2.836
C	3.614	-1.649	1.469
C	4.944	-1.305	1.774
C	2.678	-1.502	2.511
C	5.324	-0.872	3.049
H	5.704	-1.387	0.999
C	3.038	-1.055	3.784
H	1.630	-1.743	2.327
C	4.372	-0.751	4.062
H	6.366	-0.626	3.246
H	2.280	-0.946	4.557
H	4.662	-0.409	5.053
C	4.429	-2.709	-0.880
C	5.229	-3.722	-0.309
C	4.824	-2.257	-2.150
C	6.321	-4.279	-0.973
H	5.009	-4.058	0.706
C	5.922	-2.800	-2.828
H	4.286	-1.442	-2.633
C	6.671	-3.823	-2.248
H	6.909	-5.058	-0.491
H	6.194	-2.414	-3.808
H	7.524	-4.248	-2.771
C	-3.017	-3.947	1.018
C	-3.370	-3.786	2.369
C	-3.598	-5.043	0.348
C	-4.237	-4.667	3.024

H	-2.974	-2.944	2.936
C	-4.464	-5.933	0.988
H	-3.368	-5.199	-0.706
C	-4.787	-5.748	2.335
H	-4.487	-4.502	4.070
H	-4.891	-6.766	0.433
H	-5.465	-6.434	2.837
C	-2.250	-2.900	-1.351
C	-3.560	-2.622	-1.797
C	-1.284	-3.103	-2.351
C	-3.882	-2.532	-3.150
H	-4.351	-2.485	-1.058
C	-1.592	-3.013	-3.715
H	-0.261	-3.365	-2.078
C	-2.893	-2.722	-4.121
H	-4.904	-2.307	-3.448
H	-0.814	-3.188	-4.457
H	-3.139	-2.651	-5.178
C	-4.429	2.709	0.880
C	-5.229	3.722	0.309
C	-4.824	2.257	2.150
C	-6.321	4.279	0.974
H	-5.009	4.058	-0.706
C	-5.922	2.800	2.828
H	-4.286	1.442	2.633
C	-6.670	3.823	2.248
H	-6.909	5.058	0.492
H	-6.194	2.414	3.809
H	-7.524	4.248	2.772
C	-3.614	1.648	-1.469
C	-4.944	1.306	-1.775
C	-2.677	1.501	-2.510
C	-5.323	0.873	-3.050
H	-5.705	1.389	-1.001
C	-3.037	1.053	-3.783
H	-1.629	1.740	-2.326
C	-4.371	0.751	-4.062
H	-6.365	0.629	-3.248
H	-2.278	0.943	-4.556
H	-4.661	0.408	-5.054

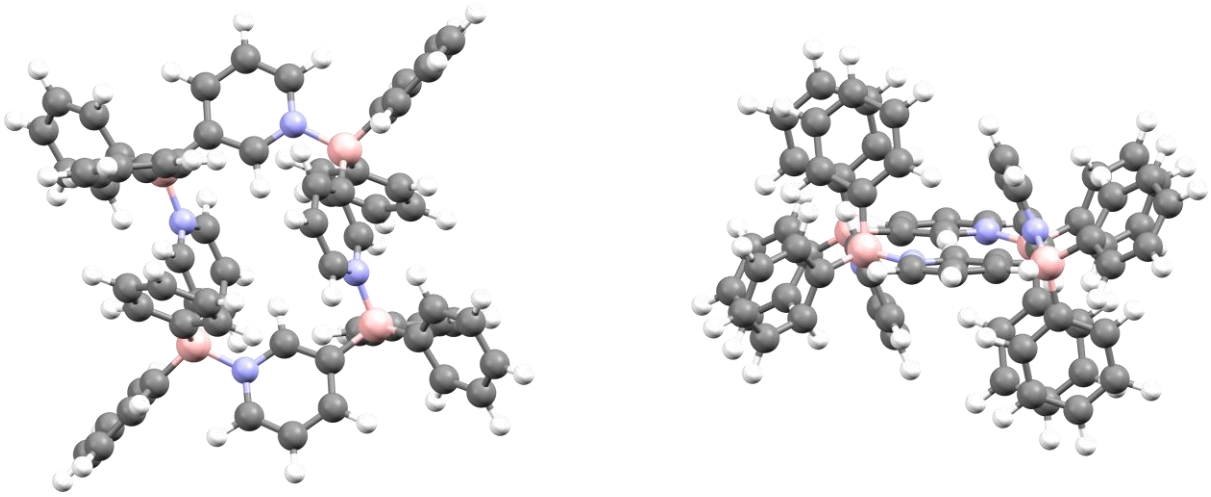

Figure S12 Two views of the optimized structure of **3**-phenyl.

Table S11 Atomic coordinates for the optimized structure of **3**-2,6-dimethylbenzene.

Atom Type	X	Y	Z Coordinates
N	-2.613	-0.793	-0.805
N	-0.337	3.562	-0.474
C	-2.571	0.461	-0.310
C	-1.891	1.524	-0.913
C	-1.135	1.169	-2.037

C	-1.139	-0.127	-2.548
C	-1.923	-1.075	-1.922
C	0.714	2.734	-0.242
C	2.071	3.098	-0.250
C	2.268	4.477	-0.435
C	1.220	5.330	-0.761
C	-0.069	4.838	-0.805
B	-1.943	3.069	-0.309
B	3.362	2.014	0.019
H	-3.123	0.594	0.612
H	-0.538	1.927	-2.540
H	-0.555	-0.401	-3.422
H	-2.031	-2.087	-2.290
H	0.417	1.713	-0.018
H	3.251	4.912	-0.328
H	1.395	6.381	-0.967
H	-0.911	5.459	-1.077
N	2.614	0.793	0.806
N	0.337	-3.562	0.475
C	2.572	-0.461	0.310
C	1.891	-1.524	0.913
C	1.136	-1.170	2.037
C	1.140	0.126	2.549
C	1.924	1.074	1.923
C	-0.713	-2.734	0.243
C	-2.071	-3.098	0.251
C	-2.268	-4.477	0.437
C	-1.220	-5.330	0.764
C	0.069	-4.838	0.808
B	1.943	-3.069	0.309
B	-3.361	-2.014	-0.018
H	3.123	-0.594	-0.612
H	0.539	-1.927	2.540
H	0.557	0.400	3.423
H	2.032	2.086	2.291
H	-0.416	-1.714	0.018
H	-3.251	-4.912	0.332
H	-1.395	-6.380	0.972
H	0.911	-5.459	1.080
C	2.470	-2.981	-1.263
C	3.850	-2.668	-1.441
C	1.718	-3.172	-2.452
C	4.391	-2.468	-2.716
C	2.291	-2.963	-3.714
C	3.618	-2.591	-3.859
H	5.442	-2.204	-2.802
H	1.677	-3.116	-4.599
H	4.047	-2.417	-4.843
C	2.887	-4.178	1.138
C	3.188	-5.421	0.503
C	3.508	-3.969	2.403
C	4.023	-6.371	1.105
C	4.346	-4.938	2.971
C	4.612	-6.141	2.337
H	4.216	-7.304	0.581
H	4.805	-4.732	3.935
H	5.265	-6.879	2.792
C	4.118	1.361	-1.312
C	5.451	0.879	-1.205
C	3.544	1.320	-2.606
C	6.191	0.558	-2.350
C	4.305	1.003	-3.736
C	5.645	0.663	-3.621
H	7.217	0.214	-2.231
H	3.826	1.003	-4.712
H	6.237	0.428	-4.502
C	4.471	2.843	0.940
C	5.186	3.888	0.277
C	4.798	2.649	2.310
C	5.999	4.776	0.986
C	5.614	3.564	2.992
C	6.188	4.650	2.355
H	6.509	5.569	0.442
H	5.823	3.388	4.046
H	6.812	5.353	2.901
C	-2.887	4.178	-1.139
C	-3.506	3.970	-2.404
C	-3.187	5.421	-0.503
C	-4.344	4.939	-2.972
C	-4.022	6.371	-1.105

C	-4.610	6.141	-2.337
H	-4.802	4.734	-3.936
H	-4.215	7.304	-0.580
H	-5.263	6.880	-2.792
C	-2.472	2.981	1.263
C	-3.853	2.669	1.439
C	-1.722	3.171	2.452
C	-4.396	2.471	2.713
C	-2.297	2.964	3.714
C	-3.624	2.594	3.857
H	-5.447	2.208	2.798
H	-1.683	3.116	4.600
H	-4.055	2.422	4.840
C	-4.470	-2.843	-0.940
C	-5.185	-3.888	-0.277
C	-4.796	-2.649	-2.310
C	-5.998	-4.777	-0.987
C	-5.611	-3.565	-2.993
C	-6.186	-4.652	-2.356
H	-6.507	-5.570	-0.443
H	-5.820	-3.389	-4.046
H	-6.808	-5.355	-2.902
C	-4.118	-1.361	1.312
C	-5.451	-0.879	1.205
C	-3.543	-1.318	2.606
C	-6.191	-0.557	2.351
C	-4.304	-1.001	3.735
C	-5.644	-0.661	3.621
H	-7.217	-0.214	2.231
H	-3.825	-0.999	4.712
H	-6.236	-0.425	4.502
C	4.863	-2.573	-0.313
H	5.207	-3.570	-0.013
H	5.732	-2.003	-0.654
H	4.485	-2.090	0.591
C	0.294	-3.682	-2.490
H	0.151	-4.615	-1.936
H	-0.402	-2.965	-2.071
H	-0.010	-3.873	-3.523
C	3.390	-2.709	3.239
H	3.681	-1.810	2.688
H	2.378	-2.549	3.618
H	4.048	-2.783	4.108
C	2.674	-5.842	-0.861
H	1.667	-5.492	-1.077
H	3.318	-5.460	-1.662
H	2.666	-6.935	-0.930
C	-5.233	-4.081	1.234
H	-6.054	-3.489	1.656
H	-5.429	-5.134	1.469
H	-4.335	-3.776	1.769
C	-4.467	-1.421	-3.152
H	-4.263	-0.527	-2.565
H	-3.621	-1.578	-3.831
H	-5.333	-1.192	-3.779
C	-6.172	-0.660	-0.110
H	-5.498	-0.309	-0.895
H	-6.659	-1.569	-0.477
H	-6.946	0.103	0.022
C	-2.070	-1.554	2.836
H	-1.792	-2.614	2.800
H	-1.482	-1.025	2.080
H	-1.775	-1.161	3.815
C	-0.296	3.677	2.491
H	0.398	2.957	2.073
H	-0.150	4.610	1.938
H	0.007	3.867	3.525
C	-4.864	2.573	0.310
H	-5.733	2.003	0.649
H	-5.208	3.569	0.009
H	-4.485	2.090	-0.594
C	-3.387	2.710	-3.240
H	-2.374	2.550	-3.618
H	-3.679	1.811	-2.691
H	-4.044	2.785	-4.110
C	-2.675	5.841	0.862
H	-3.319	5.460	1.662
H	-1.667	5.490	1.079
H	-2.665	6.934	0.931
C	6.172	0.658	0.110

H	6.660	1.567	0.477
H	5.497	0.307	0.895
H	6.945	-0.105	-0.022
C	2.071	1.556	-2.837
H	1.482	1.027	-2.081
H	1.793	2.616	-2.799
H	1.776	1.164	-3.816
C	4.468	1.421	3.152
H	3.622	1.578	3.832
H	4.264	0.526	2.565
H	5.334	1.192	3.779
C	5.232	4.082	-1.234
H	5.429	5.134	-1.469
H	6.052	3.489	-1.658
H	4.334	3.777	-1.768

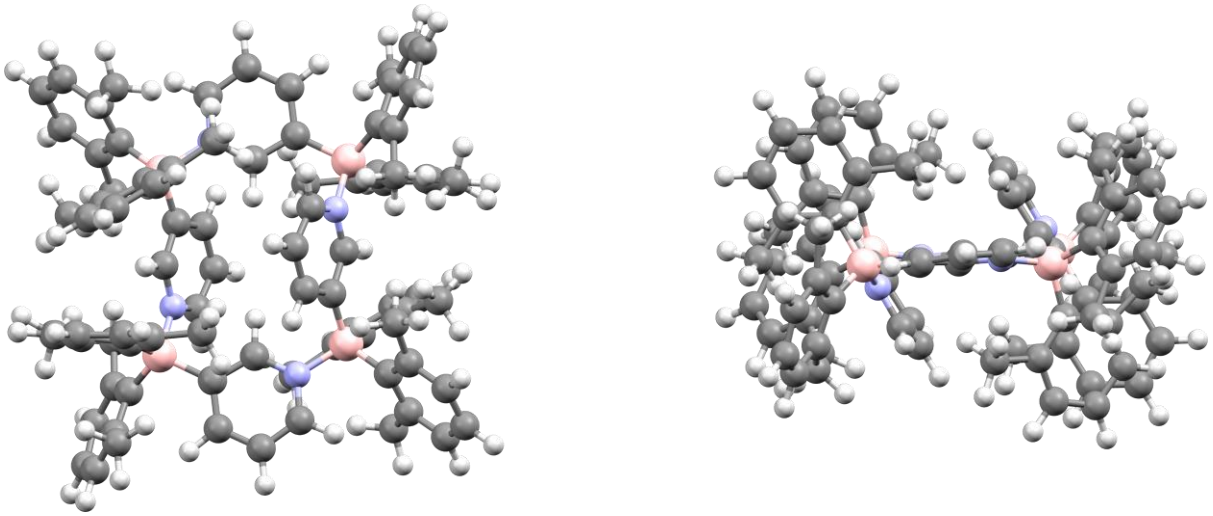

Figure S13 Two views of the optimized structure of **3**-2,6-dimethylbenzene.

Table S12 Atomic coordinates for the optimized structure of **3**-*tert*-butyl.

Atom Type	X	Y	Z Coordinates
N	1.402	-2.163	-0.633
N	-3.458	-1.449	-0.138
C	0.227	-2.555	-0.088
C	-1.039	-2.305	-0.631
C	-1.016	-1.604	-1.847
C	0.175	-1.219	-2.449
C	1.364	-1.512	-1.809
C	-2.938	-0.209	-0.013
C	-3.664	0.984	0.062
C	-5.056	0.811	0.028
C	-5.622	-0.454	-0.107
C	-4.796	-1.562	-0.194
B	-2.492	-2.804	0.008
B	-2.925	2.463	-0.008
H	0.326	-3.072	0.852
H	-1.951	-1.321	-2.323
H	0.191	-0.662	-3.380
H	2.315	-1.190	-2.207
H	-1.856	-0.188	0.030
H	-5.711	1.676	0.087
H	-6.698	-0.591	-0.143
H	-5.190	-2.564	-0.284
N	-1.402	2.163	0.633
N	3.458	1.449	0.138
C	-0.227	2.555	0.088
C	1.039	2.305	0.631
C	1.016	1.603	1.847
C	-0.176	1.219	2.448
C	-1.365	1.512	1.809

C	2.938	0.209	0.013
C	3.664	-0.984	-0.062
C	5.055	-0.811	-0.027
C	5.622	0.454	0.108
C	4.796	1.562	0.195
B	2.492	2.804	-0.007
B	2.925	-2.463	0.007
H	-0.326	3.073	-0.851
H	1.950	1.320	2.323
H	-0.193	0.662	3.380
H	-2.316	1.190	2.206
H	1.856	0.188	-0.030
H	5.711	-1.675	-0.087
H	6.697	0.591	0.145
H	5.189	2.564	0.285
C	-2.831	2.822	-1.652
C	-2.266	4.218	-2.006
C	-2.029	1.729	-2.403
C	-4.215	2.786	-2.347
H	-2.962	5.011	-1.717
H	-1.311	4.469	-1.540
H	-2.124	4.299	-3.093
H	-2.659	0.846	-2.566
H	-1.712	2.085	-3.394
H	-1.136	1.375	-1.882
H	-4.078	2.975	-3.422
H	-4.698	1.809	-2.260
H	-4.908	3.543	-1.975
C	-3.569	3.640	1.012
C	-4.044	3.096	2.379
C	-2.524	4.731	1.330
C	-4.789	4.377	0.420
H	-4.710	2.230	2.287
H	-3.212	2.815	3.033
H	-4.598	3.877	2.919
H	-2.121	5.202	0.428
H	-2.979	5.524	1.939
H	-1.676	4.335	1.903
H	-5.169	5.101	1.153
H	-4.541	4.941	-0.482
H	-5.621	3.708	0.175
C	-2.491	-3.076	1.667
C	-1.819	-1.915	2.427
C	-3.901	-3.167	2.292
C	-1.770	-4.380	2.067
H	-0.839	-1.637	2.034
H	-2.447	-1.017	2.398
H	-1.686	-2.173	3.488
H	-4.523	-3.951	1.854
H	-3.810	-3.389	3.365
H	-4.446	-2.219	2.217
H	-1.700	-4.449	3.162
H	-2.307	-5.268	1.723
H	-0.752	-4.457	1.678
C	-3.029	-4.067	-0.983
C	-4.162	-4.965	-0.436
C	-3.487	-3.601	-2.383
C	-1.845	-5.030	-1.245
H	-3.889	-5.461	0.499
H	-5.110	-4.445	-0.264
H	-4.376	-5.758	-1.166
H	-2.663	-3.179	-2.966
H	-3.859	-4.462	-2.956
H	-4.293	-2.859	-2.360
H	-2.192	-5.903	-1.816
H	-1.053	-4.555	-1.833
H	-1.390	-5.403	-0.322
C	3.569	-3.639	-1.014
C	2.524	-4.730	-1.333
C	4.044	-3.094	-2.381
C	4.789	-4.376	-0.422
H	2.122	-5.203	-0.431
H	1.676	-4.334	-1.905
H	2.979	-5.522	-1.944
H	4.709	-2.227	-2.288
H	4.598	-3.874	-2.921
H	3.212	-2.813	-3.035
H	5.170	-5.100	-1.157
H	5.621	-3.707	-0.177
H	4.542	-4.941	0.479

C	2.831	-2.823	1.651
C	2.029	-1.730	2.402
C	2.266	-4.220	2.003
C	4.214	-2.788	2.346
H	2.660	-0.849	2.567
H	1.137	-1.375	1.881
H	1.710	-2.088	3.392
H	2.963	-5.012	1.715
H	2.121	-4.301	3.090
H	1.312	-4.471	1.535
H	4.078	-2.977	3.421
H	4.908	-3.545	1.974
H	4.699	-1.811	2.259
C	2.491	3.077	-1.666
C	3.901	3.168	-2.290
C	1.820	1.916	-2.427
C	1.770	4.381	-2.065
H	4.523	3.952	-1.852
H	4.447	2.220	-2.216
H	3.811	3.391	-3.363
H	0.839	1.638	-2.034
H	1.687	2.175	-3.488
H	2.448	1.018	-2.397
H	1.700	4.450	-3.160
H	0.753	4.459	-1.676
H	2.308	5.269	-1.721
C	3.029	4.066	0.985
C	1.845	5.030	1.247
C	3.486	3.600	2.385
C	4.162	4.965	0.439
H	1.391	5.403	0.324
H	1.053	4.555	1.835
H	2.192	5.902	1.819
H	4.293	2.857	2.361
H	3.859	4.460	2.958
H	2.662	3.178	2.968
H	4.375	5.758	1.169
H	5.110	4.445	0.267
H	3.890	5.461	-0.496

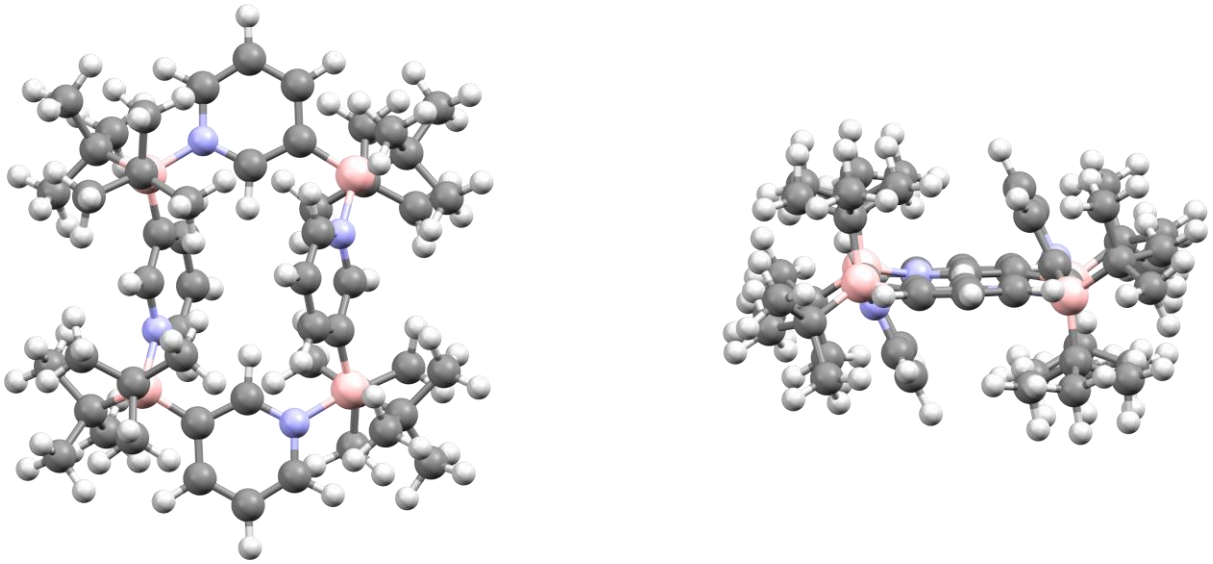

Figure S14 Two views of the optimized structure of **3**-*tert*-butyl.